

STIC Search Report Biotech-Chem Library

STIC Database Tracking Number: 150639

TO: Shailendra Kumar Location: 5c03 / 5c18 Tuesday, April 19, 2005

Art Unit: 1621

Phone: 571-272-0640 711 Serial Number: 10 / 736

From: Jan Delaval

Location: Biotech-Chem Library

Remsen 1a51

Phone: 571-272-22504

jan.delaval@uspto.gov

-Search Notes -			
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SEARCH REQUEST FORM

Location (Bldg/Room#): <u>YEM</u>	Eumar e Number: 2- 0640 (Mailbox #): 5 C18 R	Examiner # : 69590 Serial Number: 10 esults Format Preferred (c	ircle: PAPER DISK
万亡のう To ensure an efficient and quality search)	********	*****
Title of Invention: \\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\	contained to	s siect, claims, and abstract or	fill out the following:
Title of Invention:	: Johann La	ban et. of.	ry, immuno modulatory.
Earliest Priority Date: 12	22/03		·
Search Topic: Please provide a detailed statement of the se clected species or structures, keywords, synd Define any terms that may have a special m	earch topic, and describe as specij	fically as possible the subject mat mbers, and combine with the con- it citations, authors, etc., if throw	ter to be searched. Include the cept or utility of the invention.
For Sequence Searches Only Please incli appropriate serial number.	ude all pertinent information (par	rent, child, divisional, or issued po	ntent numbers) along with the
(A ^q),	$\frac{S_1}{\sum_{j=1}^{N} k_j}$	— [Dm—(C	H R ³)n]q-Y
D is 0,5, 21 & 22 are	SOD, MAY, CH	12.	
E is alkyl,	0		
Please Search Speeier of examp	a) holocology of when composed of bugge 3	etc. mid an Mon He	etemayoli'o
**************************************	******	****	
STAFF USE ONLY Searcher:	Type of Search	Vendors and cost where	applicable
Searcher Phone #: 2253 4	NA Sequence (#) AA Sequence (#)	STN	Dialog
Searcher Location:	Structure (#)	Questel/Orbit	Lexis/Nexis
Date Searcher Picked Up: 4115 (0)	Bibliographic		WWW/Internet
Date Completed: 4115(05	Litigation	In-house sequence syCommercialOligoInterference SPD	omer Score/Length

=> fil reg FILE 'REGISTRY' ENTERED AT 12:31:07 ON 19 APR 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 18 APR 2005 HIGHEST RN 848724-42-5 DICTIONARY FILE UPDATES: 18 APR 2005 HIGHEST RN 848724-42-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> d l11 ide can

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN

RN 719301-52-7 REGISTRY

ED Entered STN: 30 Jul 2004

CN 1-Cyclopentene-1-carboxylic acid, 3-hydroxy-2-[[[2,3,5,6-tetrafluoro-3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]amino]carbonyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H12 F7 N O5

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:106198

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=> d his
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(FILE 'HCAPLUS' ENTERED AT 12:26:37 ON 19 APR 2005)
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L1
                E LEBAN J/AU
L2
             60 S E3-E5, E7-E10
                E KRALIK M/AU
            120 S E3, E4
L3
                E 4SC/PA,CS
L4
             24 S E3-E20
                E 4 SC/PA,CS
L5
              2 S E5-E12
                E 4S C/PA,CS
                E 4 S C/PA, CS
              3 S L1 AND L2-L5
L6
            194 S L2-L5 NOT L6
L7
                SEL RN L6
     FILE 'REGISTRY' ENTERED AT 12:28:57 ON 19 APR 2005
L8
            164 S E1-E164
             34 S L8 AND 46.150.18/RID AND C5/ES AND 3/NR
L9
L10
              3 S L9 AND 7/F
                SEL RN 2
L11
              1 S E165
              0 S 719301-52-7/CRN
L12
     FILE 'HCAOLD' ENTERED AT 12:30:27 ON 19 APR 2005
              0 S L11
L13
     FILE 'HCAPLUS' ENTERED AT 12:30:31 ON 19 APR 2005
L14
              1 S L11
L15
              1 S L14 AND L1-L7
     FILE 'USPATFULL, USPAT2' ENTERED AT 12:30:49 ON 19 APR 2005
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FILE 'REGISTRY' ENTERED AT 12:31:07 ON 19 APR 2005

=> fil hcaplus

0 S L11

L16

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FILE COVERS 1907 - 19 Apr 2005 VOL 142 ISS 17 FILE LAST UPDATED: 18 Apr 2005 (20050418/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> d l15 all hitstr
     ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN
L15
ΑN
     2004:550930 HCAPLUS
DN
     141:106198
     Entered STN: 09 Jul 2004
ED
TI
     A preparation of cycloalkenedicarboxylic acid derivatives, useful as
     dihydroorotate dehydrogenase (DHODH) inhibitors
IN
     Leban, Johann; Kralik, Martin
PA
     4SC A.-G., Germany
so
     PCT Int. Appl., 56 pp.
     CODEN: PIXXD2
     Patent
DT
     English
LA
IC
     ICM C07C233-57
     ICS A61P035-00; A61P037-02; A61P029-00; A61P031-12; A61K031-194
     24-4 (Alicyclic Compounds)
     Section cross-reference(s): 1, 63
FAN.CNT 3
     PATENT NO.
                         KIND
                               DATE
                                           APPLICATION NO.
                                                                   DATE
     ______
                         ----
                                -----
                                            -----
PΤ
     WO 2004056746
                          A1
                                20040708
                                           WO 2003-EP14434
                                                                   20031217
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
             UG, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                           US 2003-736711
     US 2004176458
                          A1
                                20040909
                                                                   20031217 <--
     US 2004192758
                                           US 2003-736742
                          A1
                                20040930
                                                                   20031217 <--
PRAI DE 2002-10260800
                          Α
                                20021223
     US 2002-435258P
                          P
                                20021223
                                         <--
CLASS
                 CLASS PATENT FAMILY CLASSIFICATION CODES
 PATENT NO.
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 WO 2004056746
                 ICM
                        C07C233-57
                        A61P035-00; A61P037-02; A61P029-00; A61P031-12;
                 ICS
                        A61K031-194
 US 2004176458
                 ECLA
                        C07C233/58; C07C233/60; C07C235/40; C07C259/08;
                        C07D333/38
                                                                            <--
                 ECLA
                        C07D307/68; C07D333/38
US 2004192758
                                                                            <---
OS
    MARPAT 141:106198
```

GI

$$\begin{array}{c|c}
 & Z^{2} & R^{1} \\
\hline
 & N \\
 & N \\
 & R^{2}
\end{array}$$
R²

AΒ The invention relates to a preparation of cycloalkenedicarboxylic acid derivs. of formula I [wherein: A is a non-aromatic ring containing 4 to 8 carbon atoms, wherein the ring system comprises at least one double bond and wherein one or more of the carbon atoms in the ring can be replaced by S, O, N, or S(O), etc.; D is O, S, SO2, or CH2, etc.; Z1 and Z2 are independently selected from O, S, or NH, etc. ; R1 is H or alkyl; R2 is H, OH, O-(cyclo)alkyl, or NH2, etc.; R3 is H, (cyclo)alkyl, aryl, alkoxy, halogen, or O-aryl, etc.; E is an alkyl or cycloalkyl group or a (mono/poly)cyclic (un)substituted ring system; Y is H, halogen, haloalkyl, haloalkyloxy, alkyl, cycloalkyl, a monocyclic or polycyclic (un) substituted ring system; n is 0 or 1], useful as antiinflammatory, immunomodulatory and antiproliferatory agents. The obtained compds. were screened in inhibition assay for dihydroorotate dehydrogenase (DHODH) activity. For instance, cyclopentenecarboxylic acid derivative II showed IC50 value (human DHODH) of $< 1\mu M$.

ST cycloalkenedicarboxylic acid prepn antiinflammatory immunomodulator antiproliferatory agent DHODH inhibitor; dihydroorotate dehydrogenase inhibitor cycloalkenedicarboxylic acid prepn

II

IT Disease, animal

(arthropathy, treatment of; preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents)

IT Joint, anatomical

(disease, treatment of; preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents)

IT Cell proliferation

(diseases caused by malignant, treatment of; preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents)

IT Immunity

(disorder, acute, treatment of; preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents)

IT Anti-inflammatory agents Antiasthmatics

Antirheumatic agents Antiviral agents Cytotoxic agents Human Immunomodulators Protozoacides (preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents) IT Infection (protozoal, infestation, treatment of; preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents) TT Inflammation Nose, disease (rhinitis, treatment of; preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents) IT Asthma Autoimmune disease Fibrosis Inflammation Pneumocystis carinii Rheumatic diseases (treatment of; preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents) TΤ Eye, disease Inflammation (uveitis, treatment of; preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents) IT Infection (viral, treatment of; preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents) TT 59088-23-2, Dihydroorotate dehydrogenase RL: BSU (Biological study, unclassified); BIOL (Biological study) (inhibitor; preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents) IT 717824-35-6P 717824-36-7P 719301-43-6P 719301-44-7P 719301-45-8P 719301-46-9P 719301-47-0P 719301-48-1P 719301-49-2P 719301-50-5P 719301-51-6P 719301-52-7P 719301-53-8P 719301-54-9P 719301-55-0P 719301-56-1P 719301-57-2P 719301-58-3P 719301-59-4P 719301-60-7P 719301-61-8P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents) 3205-94-5 ТТ 62291-37-6 344751-62-8 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents) 31602-26-3P, 1-Cyclopentene-1,2,3-tricarboxylic acid IT 122130-99-8P 719301-42-5P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents) RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD RE (1) 4sc Ag; WO 03006425 A 2003

(2) Campaigne, E; J MED CHEM 1969, V12(2), P339 HCAPLUS

(3) Carney, R; US 4126691 A 1978 HCAPLUS

- (4) Chen, S; BIOCHEMICAL PHARMACOLOGY 1990, V40(4), P709 HCAPLUS
- (5) de Julian-Ortiz, J; JOURNAL OF MEDICINAL CHEMISTRY 1999, V42, P3308 HCAPLUS
- (6) Du Pont Pharmaceuticals Co; WO 9965867 A 1999 HCAPLUS
- (7) Eisai Co Ltd; DE 3346814 A 1984 HCAPLUS
- (8) Hauel, N; WO 03006443 A 2003 HCAPLUS
- (9) Kramer, B; WO 03006424 A 2003 HCAPLUS
- (10) Matsui; CHEMICAL ABSTRACTS + INDEXES 1976, V84(5)
- (11) Mitsubishi Chem Ind; DE 2921002 A 1979 HCAPLUS
- (12) Nippon Kayaku Kk; EP 0097056 A 1983 HCAPLUS
- (13) Sim, M; WO 0124785 A 2001 HCAPLUS
- (14) Takeda Chemical Industries; CHEMICAL ABSTRACTS + INDEXES 1981, V94(25)
- (15) Takeda Chemical Industries Ltd; DE 2851379 A 1979 HCAPLUS
- (16) Thorstensson, F; JOURNAL OF MEDICINAL CHEMISTRY 2003, V46(7), P1165 HCAPLUS
- IT 719301-52-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents)

RN 719301-52-7 HCAPLUS

CN 1-Cyclopentene-1-carboxylic acid, 3-hydroxy-2-[[[2,3,5,6-tetrafluoro-3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]amino]carbonyl]- (9CI) (CA INDEX NAME)

=> => fil reg

FILE 'REGISTRY' ENTERED AT 14:22:31 ON 19 APR 2005
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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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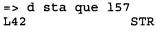
- * The CA roles and document type information have been removed from *
- * the IDE default display format and the ED field has been added,
- * effective March 20, 2005. A new display format, IDERL, is now
- * available and contains the CA role and document type information. *

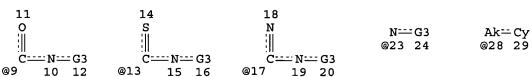
~ **********************************

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

nccp://www.cas.org/onLine/DBSS/registry





VAR G1=O/S/N
VAR G2=9/13/17/23
VAR G3=28/30
VAR G4=H/O/N
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 29
GGCAT IS UNS AT 30
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L44 2956 SEA FILE=REGISTRY SSS FUL L42

L45 STR

VAR G1=O/S/N
VAR G2=9/13/17/23
VAR G3=28/30
VAR G4=H/O/N
REP G5=(1-5) C
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GRAPH ATTRIBUTES:

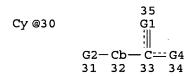
L47

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

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2423 SEA FILE=REGISTRY SUB=L44 SSS FUL L45



VAR G1=O/S/N VAR G2=9/13/17/23 VAR G3=28/30 VAR G4=H/O/N NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM **GGCAT** IS UNS AT 29 **GGCAT** IS UNS 30 ATGGCAT IS MCY AΤ 32 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L57 2097 SEA FILE=REGISTRY SUB=L47 SSS FUL L55

100.0% PROCESSED 2423 ITERATIONS

2097 ANSWERS

SEARCH TIME: 00.00.01

=> d his

L26

STR L24

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(FILE 'HCAPLUS' ENTERED AT 12:26:37 ON 19 APR 2005)
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L1
                E LEBAN J/AU
L2
             60 S E3-E5, E7-E10
                E KRALIK M/AU
L3
            120 S E3, E4
                E 4SC/PA,CS
             24 S E3-E20
L4
                E 4 SC/PA,CS
L5
              2 S E5-E12
                E 4S C/PA,CS
                E 4 S C/PA,CS
L6
              3 S L1 AND L2-L5
L7
            194 S L2-L5 NOT L6
                SEL RN L6
     FILE 'REGISTRY' ENTERED AT 12:28:57 ON 19 APR 2005
L8
            164 S E1-E164
L9
             34 S L8 AND 46.150.18/RID AND C5/ES AND 3/NR
L10
              3 S L9 AND 7/F
                SEL RN 2
L11
              1 S E165
L12
              0 S 719301-52-7/CRN
     FILE 'HCAOLD' ENTERED AT 12:30:27 ON 19 APR 2005
L13
              0 S L11
     FILE 'HCAPLUS' ENTERED AT 12:30:31 ON 19 APR 2005
L14
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L15
              1 S L14 AND L1-L7
     FILE 'USPATFULL, USPAT2' ENTERED AT 12:30:49 ON 19 APR 2005
L16
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     FILE 'REGISTRY' ENTERED AT 12:31:07 ON 19 APR 2005
     FILE 'HCAPLUS' ENTERED AT 12:31:15 ON 19 APR 2005
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L17
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L24
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L37
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L39
L40
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L42
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L44
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L45
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L46
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L47
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L48
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L49
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L50
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L51
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L52
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L53
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L54
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L55
L56
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L57
                SAV L57 KUMAR736B/A
L58
             33 S L52 AND L57
L59
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L60
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L61
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L62
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L63
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            281 S L63 NOT (PMS/CI OR SQL/FA)
L64
            169 S L64 NOT (C5-C6 OR C6-C6)/ES
L65
            146 S L65 NOT C5-C6-C6/ES
L66
L67
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L68
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L69
             24 S L67 AND (C15H13NO3 OR C16H17NO3 OR C24H22N2O2 OR C15H12CLNO3
L70
L71
             8 S L67 AND (C24H22N2O2 OR C21H18N2O2 OR C24H22N2O2 OR C17H19NO2
L72
             47 S L68-L71
             45 S L72 NOT ?NITRO?/CNS
L73
                SEL RN 34 35
L74
             43 S L73 NOT E166-E167
L75
             76 S L61, L74
            283 S L63 NOT L75
L76
             11 S L76 AND (C19H19NO4 OR C19H16N2O2 OR C23H21NO3 OR C21H20N2 OR
L77
L78
             10 S L77 NOT PMS/CI
L79
             86 S L75, L78
                SAV L79 KUMAR736D/A
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FILE 'HCAOLD' ENTERED AT 13:59:38 ON 19 APR 2005 0 S L79

L80

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FILE 'HCAPLUS' ENTERED AT 13:59:45 ON 19 APR 2005
L81
             30 S L79
L82
              3 S L81 AND L1-L7
L83
             29 S L81 AND (PD<=20021223 OR PRD<=20021223 OR AD<=20021223)
L84
             30 S L82, L83
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L85
              3 S L79
     FILE 'REGISTRY' ENTERED AT 14:01:57 ON 19 APR 2005
L86
                STR L55
     FILE 'HCAPLUS' ENTERED AT 14:05:13 ON 19 APR 2005
L87
            477 S L62
            447 S L87 AND (PY<=2002 OR PRY<=2002 OR AY<=2002)
L88
L89
             21 S L62 (L) THU/RL
              9 S L62 (L) (DMA OR PKT OR PAC)/RL
L90
L91
             62 S L62 (L) BAC/RL
             84 S L62 (L) BIOL/RL
L92
             84 S L62 (L) BIOL+NT/RL
L93
             81 S L88 AND L89-L93
L94
             47 S L88 AND (PHARMACEUT? OR PHARMACOL? OR PATHOL? OR IMMUN?)/SC,S
L95
L96
             19 S L88 AND (DISEAS? OR THERAP?)
L97
              3 S L88 AND ?DEHYDROGENASE?
     FILE 'REGISTRY' ENTERED AT 14:08:04 ON 19 APR 2005
L98
              4 S DIHYDROOROTATE DEHYDROGENASE/CN
     FILE 'HCAPLUS' ENTERED AT 14:08:12 ON 19 APR 2005
L99
              1 S L98 AND L88
              1 S L88 AND DHODH
T-100
L101
             10 S L88 AND (INFECTION+OLD, NT, PFT, RT OR INFLAMMATION+OLD, NT, PFT, R
              4 S L88 AND (IMMUNITY+OLD, NT, PFT, RT OR NOSE, DISEASE+OLD, NT, PFT, R
L102
              3 S L88 AND (FIBROSIS+OLD, NT, PFT, RT OR PNEUMOCYSTIS CARINII+OLD, N
L103
L104
            113 S L94-L97, L99-L103
             89 S L104 AND P/DT
L105
L106
             43 S L105 AND US/PC, PRC, AC
L107
             20 S L106 AND US/PC.B, PRC.B, AC.B
                SEL HIT RN
     FILE 'REGISTRY' ENTERED AT 14:14:17 ON 19 APR 2005
             51 S E168-E218
L108
L109
             12 S L108 AND (C17H23NO2 OR C15H19NO2 OR C19H23CLFNO4 OR C14H13F2N
     FILE 'HCAPLUS' ENTERED AT 14:19:15 ON 19 APR 2005
L110
             25 S L109
L111
             22 S L110 AND (PY<=2002 OR PRY<=2002 OR AY<=2002)
L112
             10 S L111 AND P/DT
L113
              8 S L112 NOT HERBICID?
L114
             23 S L106 NOT L107
                SEL HIT RN
     FILE 'REGISTRY' ENTERED AT 14:20:44 ON 19 APR 2005
L115
            330 S E219-E548
     FILE 'HCAPLUS' ENTERED AT 14:21:57 ON 19 APR 2005
L116
             38 S L84, L113
L117
              3 S L116 AND L1-L7
L118
             35 S L116 NOT L117
     FILE 'REGISTRY' ENTERED AT 14:22:31 ON 19 APR 2005
```

=> fil hcaplus

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FILE COVERS 1907 - 19 Apr 2005 VOL 142 ISS 17 FILE LAST UPDATED: 18 Apr 2005 (20050418/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l118 bib abs hitstr retable tot

L118 ANSWER 1 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:354698 HCAPLUS

DN 140:375071

- TI Asymmetric catalytic hydrogenation process for preparation of chiral cyclic β -aminoesters
- IN Deerberg, Joerg; Mcleod, Douglas D.; Yue, Tai-yuen
- PA Bristol-Myers Squibb Company, USA
- SO U.S. Pat. Appl. Publ., 18 pp. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

1	CIVI				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004082795	A1	20040429	US 2003-660345	20030911 <
	US 6835841	B2	20041228		
PRAI	US 2002-410897P	P	20020913	<	
OS GI	CASREACT 140:375071	; MARPA	T 140:3750	71	

ΙI

AB A catalytic asym. hydrogenation process of an β -enamino ester to I [B = 4-7-membered non-aromatic carbocyclic or heterocyclic ring; R1 = Q,

alk(en/yn)ylene; R2 = Q, alk(en/yn)ylene, etc.; Q = H, carbocycle, heterocycle; R3 = H, Cl, F, alk(en/yn)yl, Ph, etc.; R4 = H, alk(en/yn)yl; R5 = alkyloxy, carboxy] is described. For example, Et (R)-2-[(1-phenylethyl)amino]-1-cyclohexene-1-carboxylate is reduced (EtOH, HOAc, H2-PtO2, 17.5 bar, 40°, 16 h) to give the syn- β -amino ester which is converted to the HBr salt (>99% diastereomeric excess) and debenzylated (MeOH, H2-Pd/C, 7 bar, 40°, 16 h) to give II isolated as the HBr salt. Seven examples are described. The current process gives increased selectivity, higher yields and is more economical than prior art methods. I are useful as intermediates for MMP and TACE inhibitors.

IT 121506-74-9 683774-02-9 683774-03-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. catalytic hydrogenation process for preparation of chiral cyclic

beta-aminoesters)

RN 121506-74-9 HCAPLUS

Absolute stereochemistry.

RN 683774-02-9 HCAPLUS

CN 1-Cyclopentene-1-carboxylic acid, 2-[[(1R)-1-phenylethyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 683774-03-0 HCAPLUS

Absolute stereochemistry.

L118 ANSWER 2 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

2004:331784 HCAPLUS AN

DN 140:339193

Preparation of indole nitriles as cysteine protease, in particular ΤI Cathepsin K inhibitors

Bamberg, Joe Timothy; Gabriel, Tobias; Krauss, Nancy Elisabeth; Mirzadegan, Taraneh; Palmer, Wylie Solang; Smith, David Bernard IN

PΑ Roche Palo Alto, LLC, USA

U.S. Pat. Appl. Publ., 141 pp., Cont.-in-part of U.S. Ser. No. 308,963. SO CODEN: USXXCO

DT Patent

LA English

FAN.	CNT 2 PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡÏ	US 2004077646	A1	20040422	US 2003-453112	20030602 <
	US 6759428	B2	20040706		
	US 2003212097	A1	20031113	US 2002-308963	20021203 <
	US 6747053	B2	20040608		
PRAI	US 2001-336750P	P	20011204	<	
	US 2002-308963	A2	20021203	<	
os	MARPAT 140:339193				

GI

AB Title compds. I [wherein n = 0-2; R1 = (un)substituted indolyl, indazolyl, benzothiazolyl, indolizinyl, tetrahydropyridoindolyl; benzopyrrolothiazolyl; X = [CH(R5R6)]q; q = 1-2; R2, R3, R4, R5 =independently H, alkyl; R6 = H, cyclo/alkyl, (CRaRb)oA; Ra, Rb = independently H, alkyl; o = 0-4; A = OH and derivs., (un) substituted Ph, pyridyl, imidazolyl, morpholinyl, CO2H and derivs., etc.; Y = (CH2) m; m = 1-3; their pharmaceutically acceptable salts, solvates and prodrugs] were prepared as cysteine protease, in particular Cathepsin K inhibitors. The compds. are useful for the treatment of diseases which are associated with cysteine proteases such as osteoporosis, tumor metastasis, unstable angina pectoris and/or plaque rupture. Thus, Et (1R,2S)-2aminocyclohexanecarboxylate-HBr was treated with indole-2-carboxylic acid, followed by ester hydrolysis and amidation with (R,S)amino(cyclopropyl)acetonitrile to give the amide II. I selectively inhibited Cathepsin K (no data).

IT 680569-13-5, 2-Benzylamino-4-methylcyclohex-1-ene-1-carboxylic acid ethyl ester

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of indole nitriles as cysteine protease, in particular Cathepsin K inhibitors)

RN 680569-13-5 HCAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 4-methyl-2-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RETABLE

Referenced Author (RAU)	Year	VOL	PG (RPG)	Referenced Work (RWK)	Referenced File
	+=====:		/	+======================================	 +========
Anon	ĺ	ĺ	ĺ	ĺ	ĺ
Anon	1977	j	j	DE 2624290 A1	HCAPLUS
Anon	1998	İ	İ	WO 9803540 A2	HCAPLUS
Anon	1999	İ	i	WO 9924460 A2	HCAPLUS
Anon	2001	İ	İ	WO 0149288 A1	HCAPLUS
Anon	2001	İ		WO 0196285 A1	HCAPLUS
Anon	2003	İ	Ì	WO 03041649 A2	HCAPLUS
Broemme	1999	12	73	Drug News Perspect	
Chapman	1997	59	63	Annu. Rev. Phys	HCAPLUS
Davies	1994	1	1411	J. Chem. Soc. Perkin	
Everts	1992	150	221	J. Cell. Physiol	HCAPLUS
Gabriel	2002			US 6462076 B2	HCAPLUS
Hummel	1998	25:10	1887	J. Rheumatol.	
Kobayashi	1990	38:2	350	Chem. Pharm. Bull.	
Lerner	1992	7:4	433	J. Bone Min Res.	
Littlewood-Evans	1997	57	5386	Cancer Res	HCAPLUS
Maubach	1997	250:2	745	Eur. J. Biochem.	
Otto	1997	97	133	Chem. Rev	HCAPLUS
Rink	1987	28:33	3787	Tetrahedron Lett.	
Schaper	1997	ļ		US 5691321 A	HCAPLUS
Sukhova	1998	102:3	!	J. Clin. Invest.	
Tezuka	1994	269	1106	J. Biol. Chem.	HCAPLUS
Thompson	1997	94	14249	Proc. Natl. Acad. Sc	HCAPLUS

L118 ANSWER 3 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:269913 HCAPLUS

DN 140:287277

TI Preparation of carboxylic acid derivatives that inhibit the binding of integrins to their receptors

IN Biediger, Ronald J.; Chen, Qi; Decker, E. Radford; Holland, George W.;
Kassir, Jamal M.; Li, Wen; Market, Robert V.; Scott, Ian L.; Wu, Chengde;
Li, Jian

PA USA

SO U.S. Pat. Appl. Publ., 98 pp., Cont.-in-part of U.S. Ser. No. 707,068. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 3

I FIIV.	PATENT NO.	KIND DATE		APPLICATION NO.	DATE			
PΙ	US 2004063955	A1	20040401	US 2001-973142	20011009 <			
	ZA 2001008777	Α	20030124	ZA 2001-8777	20011024 <			
	NZ 515252	A	20040130	NZ 2001-515252	20011102 <			
	NO 2001005394	A	20020507	NO 2001-5394	20011105 <			
	EP 1203766	A2	20020508	EP 2001-125494	20011106 <			
	EP 1203766	A3	20041208					
	R: AT, BE, CH,	DE, DK	, ES, FR,	GB, GR, IT, LI, LU, NL,	SE, MC, PT,			
	IE, SI, LT,	LV, FI	, RO, MK,	CY, AL, TR				
	TR 200103179	A2	20020621	TR 2001-200103179	20011106 <			
	BR 2001006840	Α	20050201	BR 2001-6840	20011106 <			
	CN 1412181	A	20030423	CN 2001-145182	20011229 <			
	CA 2366800	AA	20030410	CA 2002-2366800	20020107 <			
	JP 2003119181	A2	20030423	JP 2002-31953	20020208 <			
PRAI	US 1999-132971P	P	19990507	<				
	US 2000-565920	A2	20000505	<				
	US 2000-707068	A2	20001106	<				
	US 2001-973142	A	20011009	<				
os GI	MARPAT 140:287277							

The invention relates to a method for the inhibition of the binding of α4β1 integrin to its receptors [e.g., VCAM-1 (vascular cell adhesion mol.-1) and fibronectin], compds. that inhibit this binding, and the use of such compds. for the control or prevention of diseases states in which α4β1 is involved. The claims include compds. of general formula I [n is 3-10; Y is CO, N, CR1, CR2R3, NR5, CH, O, S; A is O, S, CR16R17, NR6; E is CH2, O, S, NR7; J is O, S, NR8; T is CO, (CH2)0-3; M is R9R10, (CH2)0-3; L is O, NR11, S, (CH2)0-1; X is CO2B, PO3H2, SO3H, SO2NH2, SO2NHCOR12, OPO3H2, CONHCOR13, CONHSO2R14, OH, tetrazolyl, H; W is C, CR15, N; B, R1-R17 are H, halo, alkyl, alkoxy, acyl, CF3, CO2H, etc.]. Thus, pyridine-containing 3-aminopropionic acid derivative II was prepared by a multistep procedure and showed IC50 = 10 nM in

fibronectin inhibition assay.

IT 422519-80-0P

а

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of carboxylic acid derivs. that inhibit the binding of integrins to their receptors)

RN 422519-80-0 HCAPLUS

CN 1-Cyclopentene-1-carboxylic acid, 2-[[(2-chlorophenyl)methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

L118 ANSWER 4 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:183000 HCAPLUS

DN 140:199750

TI Heterogeneous foldamers containing α , β and/or γ -amino acids

```
Gellman, Samuel H.; Hayen, Ahlke; Schmitt, Margaret A.; Ngassa, Felix N.
     Wisconsin Alumni Research Foundation, USA
PA
     PCT Int. Appl., 149 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
                         _ _ _ _
                                             ______
                                             WO 2003-US26694
                                                                     20030826 <--
PΙ
     WO 2004018644
                          A2
                                 20040304
     WO 2004018644
                          A3
                                 20040701
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                          A1
                                 20040617
                                          US 2003-648089
     US 2004116654
                                                                     20030826 <--
PRAI US 2002-406006P
                          P
                                 20020826 <--
     Disclosed are isolated, unnatural polypeptides A-(Xa-Y-Zc)d-A [X, Z are
     \alpha-, \beta-, or \gamma-amino acid residues, provided that at least
     one X or Z is an \alpha-amino acid residue and at least two of X or Z are
     cyclically-constrained \gamma-amino acid residues; Y is a single bond or
     a reverse-turn moiety; A is H, OH, an amino or carboxy protecting group;
     a, c, and d are pos. integers, where a + c > 3] or their salts. The
     compds. are useful for probing protein-protein and other large mol.
     interactions, since they are not amenable to enzymic degradation. The examples
     describe syntheses of peptides of the invention, including
     Boc-D-Ala-ACHC-OBn, where ACHC is the \beta-amino acid
     trans-2-aminocyclohexanecarboxylic acid.
IT
     121506-74-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (heterogeneous foldamers containing \alpha, \beta, and/or \gamma-amino
        acids)
RN
     121506-74-9 HCAPLUS
     1-Cyclohexene-1-carboxylic acid, 2-[[(1R)-1-phenylethyl]amino]-, ethyl
CN
     ester (9CI) (CA INDEX NAME)
```

Absolute stereochemistry.

L118 ANSWER 5 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:349146 HCAPLUS

DN 136:369608

TI Preparation of 3-(N'-oxodihydropyridinylureido)-3-phenylpropanoates as inhibitors of $\alpha 4\beta 1$ integrin binding

IN Biediger, Ronald J.; Chen, Qi; Holland, George W.; Kassir, Jamal M.; Li, Wen; Market, Robert V.; Scott, Ian L.; Wu, Chengde; Decker, Radford E.; Li, Jian

PA Texas Biotechnology Corporation, USA

SO Eur. Pat. Appl., 131 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 3

	PATENT NO.					KIND DATE		A	APPLICATION NO.					DATE					
ΡI	EP	1203	766			A2	•	2002	0508	- E	 P 2	001-	 1254:	 94		2	0011	106	<
		1203	. 1			A3			1208	_		••-							
		R:	ΑT,	ΒE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	,
			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR							
	US	2004	0639	55		A1		2004	0401	U	S 2	001-	9731	42		2	0011	009	<
	ZA	2001	0087	77		Α		2003	0124	Z	A 2	001-	8777			2	0011	024	<
	BR	2001	00684	40		Α		2005	0201	В	R 2	001-	6840			2	0011	106	<
PRAI	US	2000	-707	068		Α		2000	1106	<									
	US	2001	-973	142		Α		2001	1009	<									
	US	1999	-132	971P		P		1999	0507	<									
	US	2000	-565	920		A2		2000	0505	<									
00	147.1	שמחכ	120.	2000	^ ^														

OS MARPAT 136:369608

AB Title compds. were prepared Thus, 2-ClC6H4CH2ZNH2 (Z = 4-ethyl-2-oxo-1,2-dihydropyridine-1,3-diyl) (preparation given) was condensed with

(S)-4-MeC6H4CH(NH2)CH2CO2Et and COCl2 to give, after saponification,

(S)-2-ClC6H4CH2ZNHCONHCH(C6H4Me-4)CH2CO2H (Z as above). Data for biol. activity of title compds. were given.

IT 422519-80-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 3-(N'-oxodihydropyridinylureido)-3-phenylpropanoates as inhibitors of $\alpha 4\beta 1$ integrin binding)

RN 422519-80-0 HCAPLUS

CN 1-Cyclopentene-1-carboxylic acid, 2-[[(2-chlorophenyl)methyl]amino]-,
 ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 \\ \hline \\ CH_2-NH \\ \hline \\ EtO-C \\ \hline \\ O \\ \end{array}$$

L118 ANSWER 6 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:806040 HCAPLUS

DN 134:71724

TI Heteroannelations with pinane-derived β-enaminoaldehyde

AU Popov, Sergey A.; Tkachev, Alexey V.

CS Department of Natural Sciences, Novosibirsk Institute of Organic Chemistry, Siberian Branch of Russian Academy of Sciences, Novosibirsk State University, Novosibirsk, 630090, Russia

SO Heterocyclic Communications (2000), 6(4), 327-332 CODEN: HCOMEX; ISSN: 0793-0283

PB Freund Publishing House Ltd.

DT Journal

LA English

- OS CASREACT 134:71724
- AB Synthesis of new chiral fused pyridines and pyrimidines with pinane carbon frame prospective as bioactive compds. is described. Heterocyclizations of pinane-derived β -enaminoaldehyde, need generally more rigid conditions than for o-aminobenzaldehyde, probably, both due to sterical and electronic reasons.
- IT 315674-70-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(heteroannelations with pinane-derived β -enaminoaldehyde)

RN 315674-70-5 HCAPLUS

CN Benzamide, N-[(1R,5R)-2-formyl-6,6-dimethylbicyclo[3.1.1]hept-2-en-3-yl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L118 ANSWER 7 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:693187 HCAPLUS

DN 133:350683

TI Synthesis and photochemical reaction of polymers containing norbornadiene residues both in the main chain and side chain

AU Sampei, Makoto; Hiramatu, Ken; Kameyama, Atsushi; Nishikubo, Tadatomi

CS Department of Applied Chemistry, Faculty of Engineering University, Yokohama, 221-8686, Japan

SO Kobunshi Ronbunshu (2000), 57(9), 569-576 CODEN: KBRBA3; ISSN: 0386-2186

PB Kobunshi Gakkai

DT Journal

LA Japanese

The polyaddn. of 2,5-norbornadiene-2,3-dicarboxylic acid diglycidyl ester AB (NDGE) with adipoyl chloride gave a polyester (P-1) containing norbornadiene (NBD) residues in the main chain and pendant chloromethyl groups in the side chain. Polyesters containing NBD resides both in the main chain and side chains were synthesized by the polymer reaction of P-1 with certain NBD When substitution reactions of P-1 with potassium 3-phenyl-2,5-NBD-2-carboxylate (PNC), potassium 3-phenyl-2,5-NBD-2-(4'hydroxyphenyl) ketone (PNHK), potassium 3-(N,N-dipropylcarbamoyl)-2,5-NBD-2-carboxylate (DPNC), and potassium 3-(N-methyl-N-phenylcarbamoyl)-2,5-NBD-2-carboxylate (MPNC) were carried out using tetrabutylammonium bromide (TBAB) as a phase transfer catalyst in NMP for 48 h, corresponding NBD polymers (P-2-P-5) containing PNC, PNHK, DPNC, or MPNC groups were obtained in good yields. When the photochem. valence isomerization of NBD residues in polymers was performed in the film state, the rate of the photochem. reaction of NBD residue in the main chain of P-2 was higher than that of The NBD residues in the main chain of P-2 were sensitized by the pendant PNC moieties. The photo-irradiated P-2 film containing QC (quadricyclane) moieties both in the main chain and side chain released 331 J/g of thermal energy, which is the highest record as compared with other NBD polymers synthesized before.

IT 159091-04-0DP, reaction products with adipoyl chloride-2,5norbornadiene-2,3-dicarboxylic acid diglycidyl ester copolymer RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis and photochem. reaction of polymers containing norbornadiene residues both in main chain and side chain)

RN 159091-04-0 HCAPLUS

Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3[(methylphenylamino)carbonyl]-, potassium salt (9CI) (CA INDEX NAME)

CN

● ĸ

L118 ANSWER 8 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:202256 HCAPLUS

DN 130:338468

TI Synthesis and photochemical properties of poly(ester-amide)s containing norbornadiene (NBD) residues

AU Ikeda, Akihiko; Tsubata, Akinori; Kameyama, Atsushi; Nishikubo, Tadatomi

CS Department of Applied Chemistry, Faculty of Engineering, Kanagawa University, Rokkakubashi, Kanagawa-ku, Yokohama, 221-8686, Japan

SO Journal of Polymer Science, Part A: Polymer Chemistry (1999), 37(7), 917-926
CODEN: JPACEC; ISSN: 0887-624X

PB John Wiley & Sons, Inc.

DT Journal

LA English

AB N,N'-Bis[(3-carboxynorbornadien-2-yl)carbonyl]-N,N'-diphenylethyl-enediamine (BNPE) was synthesized in 70% yield by the reaction of 2,5-norbornadiene-2,3-dicarboxylic acid anhydride with N,N'-diphenylethylenediamine. Other dicarboxylic acid derivs. containing norbornadiene (NBD) residues having N,N'-disubstituted amide groups were also prepared by the reaction of 2,5-NBD-2,3-dicarboxylic acid anhydride with secondary diamines. When the polyaddn. of BNPE with bisphenol A diglycidyl ether (BPGE) was carried out using tetrabutylammonium bromide as a catalyst in N-methyl-2-pyrrolidone at 100° for 12 h, a polymer with number average mol. weight of 69,800 was obtained in 98% yield.

Polyaddns. of

other NBD dicarboxylic acid derivs. containing N,N'-disubstituted amide groups with BPGE were also performed under the same conditions. The reaction proceeded smoothly to give the corresponding NBD poly(ester-amide)s in good yields. Photochem. reactions, i.e., photoisomerization and catalytic reversion (CoTPP) of the quadricyclane groups, of the obtained polymers with N,N'-disubstituted amide groups on the NBD residue were examined, and these polymers were effectively sensitized by adding appropriate photosensitizers such as 4-(N,N-dimethylamino)benzophenone and 4,4'-bis(N,N-diethylamino)benzophenone in the film state. The stored thermal energy in the quadricyclane groups of the polymers was about 94 kJ/mol as determined from DSC measurements of irradiated polymer films.

IT 224566-45-4P, N,N'-Bis[(3-carboxynorbornadien-2-yl)carbonyl]-N,N'-diphenylethylenediamine 224566-46-5P, N,N'-Bis[(3-carboxynorbornadien-2-yl)carbonyl]-N,N'-dimethyldiaminodiphenylmethane 224566-47-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(monomer; preparation of norbornadiene-diphenyldiamine monomers and polymerization

with bisphenol-A diglycidyl ether)

RN 224566-45-4 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3,3'-[1,2-ethanediylbis[(phenylimino)carbonyl]]bis-(9CI) (CA INDEX NAME)

RN 224566-46-5 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3,3'-[methylenebis[4,1-phenylene(methylimino)carbonyl]]bis- (9CI) (CA INDEX NAME)

RN 224566-47-6 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3,3'-[oxybis[4,1-phenylene(methylimino)carbonyl]]bis- (9CI) (CA INDEX NAME)

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
=======================================	+====-	+====- ·	+=====· ·	+=====================================	
Barluenga, J	1984		1334	J Chem Soc Chem Comm	HCAPLUS
Barluenga, J	1980		1420	J Chem Soc Perkin Tr	HCAPLUS
Hautala, R	1977	19	503	Solar Energy	HCAPLUS
Hautala, R	1979		333	Solar Energy	HCAPLUS
Kamogawa, H	1992	65	2306	Bull Chem Soc Jpn	HCAPLUS
King, R	1979	44	385	J Org Chem	HCAPLUS
Maruyama, K	1981		839	Chem Lett	HCAPLUS
Maruyama, K	1981	46	5294	J Org Chem	HCAPLUS
Maruyama, K	1985	50	4742	J Org Chem	HCAPLUS
Nishibuko, T	1989	22	8	Macromolecules	
Nishibuko, T	1992	25	4469	Macromolecules	
Nishibuko, T	1994	27	1087	Macromolecules	
Nishibuko, T	1987	19	991	Polym J	
Nishibuko, T	1992	24	1165	Polym J	
Nishikubo, T	1994	32	2765	J Polym Sci Part A:	HCAPLUS

Toa Nenryo Kogyo, K	1989		1	JP 01292028	HCAPLUS
Tsubata, A	1996	53	530	Kobunshi Ronbunshu	HCAPLUS
Tsubata, A	1997	54	37	Kobunshi Ronbunshu	HCAPLUS
Tsubata, A	1997	30	6549	Macromolecules	

L118 ANSWER 9 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1997:565479 HCAPLUS

DN 127:234647

TI Synthesis of Poly(ester-amide)s Containing Norbornadiene (NBD) Residues by the Polyaddition of NBD Dicarboxylic Acid Derivatives with Bis(epoxide)s and Their Photochemical Properties

AU Tsubata, Akinori; Uchiyama, Takeshi; Kameyama, Atsushi; Nishikubo, Tadatomi

CS Department of Applied Chemistry Faculty of Engineering, Kanagawa University, Yokohama, 221, Japan

SO Macromolecules (1997), 30(19), 5649-5654 CODEN: MAMOBX; ISSN: 0024-9297

PB American Chemical Society

DT Journal

LA English

N, N'-Bis[(3-carboxynorbornadien-2-yl)carbonyl]methylenedianiline (BNMA) AB was synthesized in 87 % yield by the reaction of 2,5-norbornadiene-2,3dicarboxylic acid anhydride with 4,4'-methylenedianiline. Other dicarboxylic acid derivs. containing norbornadiene (NBD) residues were also prepared by the reaction of 2,5-NBD-2,3-dicarboxylic acid anhydride with certain diamines. When the polyaddn. of BNMA with bisphenol A diglycidyl ether (BPGE) was carried out using tetrabutylammonium bromide as a catalyst in NMP at 100° for 24 h, a polymer with a number-average mol. weight 18 000 was obtained in 91% yield. Polyaddns. of other NBD dicarboxylic acid derivs. with BPGE were also performed under the same conditions. The reaction proceeded very smoothly to give the corresponding NBD poly(ester-amide)s in good yields. Furthermore, the photochem. reactions of the NBD poly(ester-amide)s were evaluated in the film state or in solution The photochem. valence isomerization of NBD residues in the polymer films proceeded smoothly to form the corresponding quadricyclane (QC) groups upon irradiation with sunlight. The photochem. reversion of the resulting QC groups in the polymer films proceeded efficiently by irradiation of 272-nm light. The stored energy in the QC groups of the polymers was evaluated to be about 84 kJ/mol by DSC measurement of the irradiated polymer films. IT

(in synthesis of polyester-polyamine from norbornadiene-containing dicarboxylic acid derivs. with bis(epoxide)s)

RN 195303-93-6 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3,3'-[methylenebis(4,1-phenyleneiminocarbonyl)]bis-(9CI) (CA INDEX NAME)

RN 195303-94-7 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3,3'-[oxybis(4,1-phenyleneiminocarbonyl)]bis- (9CI) (CA INDEX NAME)

RN 195303-95-8 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3,3'-[(3,3'-dimethyl[1,1'-biphenyl]-4,4'-diyl)bis(iminocarbonyl)]bis- (9CI) (CA INDEX NAME)

RF		

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
77-4-1	+====:	+====- ! 0 0 5	+=====	+======================================	+======= '
Hatchard, C	1956	235	518	Proc R Soc London, S	1
Hautala, R	1977	19	503	Sol Energy	HCAPLUS
Hautala, R	1979		333	Solar Energy	HCAPLUS
Iizawa, T	1992	25	21	Macromolecules	HCAPLUS
King, R	1979	44	385	J Org Chem	HCAPLUS
Maruyama, K	1985	58	781	Bull Chem Soc Jpn	HCAPLUS
Maruyama, K	1981		839	Chem Lett	HCAPLUS
Nishikubo, T	1991	29	671	J Polym Sci, Part A:	HCAPLUS
Nishikubo, T	1994	32	2765	J Polym Sci, Part A:	HCAPLUS
Nishikubo, T	1989	22	8	Macromolecules	HCAPLUS
Nishikubo, T	1992	25	4469	Macromolecules	HCAPLUS
Nishikubo, T	1994	27	1087	Macromolecules	HCAPLUS
Nishikubo, T	1994	24	65	Reactive Polym	HCAPLUS
Nishimura, I	1996	29	3818	Macromolecules	HCAPLUS
Takamura, S	1995	52	415	Kobunshi Ronbunshu	HCAPLUS
Tsubata, A	1996	53	530	Kobunshi Ronbunshu	HCAPLUS
Tsubata, A	1997	54	37	Kobunshi Ronbunshu	HCAPLUS

L118 ANSWER 10 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1997:473696 HCAPLUS

DN 127:95206

- TI Preparation of polycyclic compounds for treatment of Alzheimer's disease
- IN Proctor, George Rennet; Harvey, Alan Lang; Mckenna, Maureen Theresa;
 Mullins, Steven John
- PA University of Strathclyde, UK; Proctor, George Rennet; Harvey, Alan Lang; Mckenna, Maureen Theresa; Mullins, Steven John
- SO PCT Int. Appl., 18 pp. CODEN: PIXXD2
- DT Patent
- LA English

FAN.CNT 1

	PATENT NO.					KIND		DATE			APPLICATION NO.					DATE			
							-												
ΡI	WO 9719929			A 1		1997	0605	1	WO 1:	996-0	GB29	45		1:	9961	128	<		
		W:	ΑL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,	
			DK,	EE,	ES,	FI,	GB,	GE,	HU,	IL,	IS,	JP,	KE,	KG,	ΚP,	KR,	KZ,	LC,	

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LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT,
             RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN,
             AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR,
             IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML,
             MR, NE, SN,
                         TD, TG
     AU 9677027
                           A1
                                 19970619
                                             AU 1996-77027
                                                                      19961128 <--
                                             EP 1996-940019
                                                                      19961128 <--
     EP 877735
                           A1
                                 19981118
         R:
             CH, DE, FR,
                         GB,
                              IT, LI, NL
                                 20000202
                                             JP 1997-520287
                                                                      19961128 <--
     JP 2000501092
                           T2
                                             US 1998-77453
                                                                      19980825 <--
     US 6130228
                           Α
                                 20001010
PRAI GB 1995-24346
                           Α
                                 19951129
                                            <--
     WO 1996-GB2945
                           W
                                 19961128
                                           <--
os
     MARPAT 127:95206
GΙ
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AB The title compds. [I; R1 = NH2, OH, H, etc.; R2 = H, halo, OH, etc.; R3, R4 = H, halo, MeO, etc.; R5 = H, halo, NO2, etc.; X = (CH2)n (wherein n = 1-4); Y = (CH)m, (CH2)m (wherein m = 1-3); A = C(NHR9) (wherein R9 = H, C1-6 alkyl, aryl); ring B = (un)saturated ring optionally fused to ring C at any face of ring C; ring C is optionally substituted by one or more groups selected from H, C1-6 alkyl, COOH, COOC1-6alkyl] which exhibit anti-acetylcholinesterase activity and/or inhibition of 5-HT uptake and/or inhibition of noradrenaline uptake, were prepared Thus, reaction of 3,5-difluoroaniline with 2-oxocyclopentanecarbonitrile in the presence of CaCl2 in THF followed by cyclization of the intermediate II in the presence of TiCl4 afforded the polycyclic compound III which showed IC50 of 0.120 μM against acetylcholinesterase (AChE) and IC50 of 1.400 μM against butyrylcholinesterase (BChE).

Ι

IT 52909-66-7P

RN

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of polycyclic compds. for treatment of Alzheimer's disease). 52909-66-7 HCAPLUS

CN 1-Cyclopentene-1-carboxylic acid, 2-(phenylamino)-, ethyl ester (9CI) (CA INDEX NAME)

L118 ANSWER 11 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:287658 HCAPLUS

DN 122:82267

TI Synthesis and photochemical properties of insoluble polystyrene beads containing pendant norbornadiene moieties

AU Nishikubo, Tadatomi; Kameyama, Atsushi; Kishi, Katsuhiko; Hijikata, Chikara

CS Department of Applied Chemistry, Faculty of Engineering, Kanagawa University, Rokkakubashi, Kanagawa-ku, Yokohama, 221, Japan

SO Reactive Polymers (1994), 24(1), 65-72 CODEN: REPLEN; ISSN: 0923-1137

PB Elsevier

DT Journal

LA English

AB Insol. polymer beads bearing pendant norbornadiene moieties were prepared by reacting insol. chloromethylated polystyrene beads with K salts of norbornadiene derivs. containing carboxylic or phenolic groups using a phase transfer catalyst. The reaction proceeded smoothly in high conversion in DMF at 90° for 72 h. The rates of photochem. reaction of the norbornadiene group-containing polymers were measured by IR spectrometry. The photochem. valence isomerization of the 3-phenyl-2,5-norbornadiene-2-carboxylate derivative to the corresponding quadricyclane derivative and the reverse reaction were examined in CH2Cl2, and the reactions were carried out in high conversion over 10 cycles.

137895-90-0DP, Potassium 3-(phenylcarbamoyl)-2,5-norbornadiene-2carboxylate, reaction products with chloromethylated polystyrene
137895-92-2DP, Potassium 3-[(4-methoxyphenyl)carbamoyl]-2,5norbornadiene-2-carboxylate, reaction products with chloromethylated
polystyrene 159091-04-0DP, Potassium 3-(methylphenylcarbamoyl)2,5-norbornadiene-2-carboxylate, reaction products with chloromethylated
polystyrene

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, properties and photochem. isomerization of insol. norbornadiene group-containing polystyrene beads as energy storage materials)

RN 137895-90-0 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl], monopotassium salt (9CI) (CA INDEX NAME)

K

RN 137895-92-2 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-methoxyphenyl)amino]carbonyl]-, monopotassium salt (9CI) (CA INDEX NAME)

K

RN 159091-04-0 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3[(methylphenylamino)carbonyl]-, potassium salt (9CI) (CA INDEX NAME)

K

L118 ANSWER 12 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:254478 HCAPLUS

DN 122:32296

TI Synthesis of rigid polymer containing pendant norbornadiene moieties and its photochemical valence isomerization

AU Iizawa, Takashi; Sueyoshi, Tomoko; Hijikata, Chikara; Nishikubo, Tadatomi

CS Department Chemical Engineering, Hiroshima University, Higashi-Hiroshima, 724, Japan

SO Journal of Polymer Science, Part A: Polymer Chemistry (1994), 32(16), 3091-8

CODEN: JPACEC; ISSN: 0887-624X

PB Wiley

DT Journal

LA English

AB Polymers having pendant norbornadiene (NBD) groups on a rigid main chain were prepared by reacting partially brominated poly(2,6-dimethyl-p-phenylene oxide) with the K salt of a 2,5-norbornadiene-2-carboxylate derivative using a phase transfer catalyst in chlorobenzene. The photochem. valence isomerization of the pendant NBD to quadricyclane (QC) groups proceeded smoothly in the film state as in solution by UV irradiation. The rate of isomerization was affected by the structure of the main chain in the polymer and the substituent groups on NBD. The catalytic reversion of the resulting QC group to the original NBD proceeded smoothly in the presence of (5,10,15,20-tetraphenyl-21H,23H-porphine)cobalt(II) at room temperature 137895-90-0DP, Potassium 3-(phenylcarbamoyl)-2,5-norbornadiene-2-carboxylate, reaction products with brominated poly(dimethylphenylene oxide)

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and photochem. valence isomerization of polyoxyphenylenes containing pendant norbornadiene groups)

RN 137895-90-0 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-, monopotassium salt (9CI) (CA INDEX NAME)

K

L118 ANSWER 13 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1994:681340 HCAPLUS

DN 121:281340

TI Synthesis and photochemical properties of solar energy storage-exchange polymers containing pendant norbornadiene moieties

AU Nishikubo, Tadatomi; Kameyama, Atsushi; Kishi, Katsuhiko; Mochizuki, Yasushi

CS Fac. Eng., Kanagawa Univ., Yokohama, 221, Japan

SO Journal of Polymer Science, Part A: Polymer Chemistry (1994), 32(14), 2765-73
CODEN: JPACEC; ISSN: 0887-624X

DT Journal

LA English

AB New photoresponsive polymers (PRP) containing pendant norbornadiene (NBD) moieties with N,N-disubstituted amide groups were synthesized with 97, 98, 92, and 94% conversions by the substitution reaction of poly[(p-chloromethyl)styrene] with potassium salts of 3-piperidyloxo-2,5-NBD-2-carboxylic acid, 3-(N,N-dipropylcarbamoyl)-2,5-NBD-2-carboxylic acid, and 3-(N,methyl-N-phenylcarbamoyl)-2,5-NBD-2-carboxylic acid, and 3-(N,N-diphenylcarbamoyl)-2,5-NBD-2-carboxylic acid, resp., using tetrabutylammonium bromide as a phase-transfer catalyst for all. Polymers PRP with N,N-disubstituted amide groups on the NBD moieties were

sensitized by adding appropriate photosensitizers such as Michler's ketone and 4-(N,N-dimethylamino) benzophenone in the film state, although the reactivities of the polymers without photosensitizer were lower than that of our previously reported polymer containing pendant 3-(N-phenylcarbamoyl)-2,5-NBD-2-carboxylate moiety. The photo-irradiated retaining PRP containing the corresponding quadricyclane moieties can be stored about 80-86 kJ/mol of their thermal energy.

IT 78941-78-3P 98736-27-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; in preparation of solar energy storage-exchange polymers containing pendant norbornadiene moieties containing amide groups without imidization side reaction)

RN 78941-78-3 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl](9CI) (CA INDEX NAME)

RN 98736-27-7 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(methylphenylamino)carbonyl]- (9CI) (CA INDEX NAME)

RN 137895-90-0 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl], monopotassium salt (9CI) (CA INDEX NAME)

■ 14

RN 159091-04-0 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3[(methylphenylamino)carbonyl]-, potassium salt (9CI) (CA INDEX NAME)

● к

L118 ANSWER 14 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1994:580326 HCAPLUS

DN 121:180326

TI New photoresponsive polymers bearing norbornadiene moiety. Synthesis by selective cationic polymerization of 2-(3-phenyl-2,5-norbornadiene-2-carbonyloxy)ethyl vinyl ether and photochemical reaction of the resulting polymers

AU Nishikubo, T.; Kameyana, A.; Kishi, K.; Hijikata, C.

CS Fac. Eng., Kanagawa Univ., Yokohama, 221, Japan

SO ACS Symposium Series (1994), 537(Polymer for Microelectronics), 356-69
CODEN: ACSMC8; ISSN: 0097-6156

DT Journal

LA English

AB New functional monomers such as 2-(3-phenyl-2,5-norbornadien-2-ylcarbonyloxy)ethyl vinyl ether (PNVE), 2-[3-(phenylcarbamoyl)-2,5-norbornadien-2-ylcarbonyloxy]ethyl vinyl ether (PCNVE), 2-(4-vinylbenzyloxycarbonyl)-3-phenyl-2,5-norbornadiene (VPNB), and 2-(4-vinylbenzyloxycarbonyl)-3-(phenylcarbamoyl)-2,5-norbornadiene (VPCNB) containing both polymerizable vinyl groups and photoresponsive norbornadiene (NBD) moieties were synthesized in high yields by the reaction of K 2,5-norbornadiene-2-carboxylates with 2-chloroethyl vinyl ether or p-(chloromethyl)styrene using a phase-transfer catalyst. Although cationic polymerization or copolymn. of PNVE proceeded successfully to give soluble

polymers bearing NBD moieties in high yield without any gel products at -10 and -40° in CH2Cl2 solution, the cationic polymerization of PCNVE and VPCNB did not occur under similar conditions. Radical polymerization or

copolymn. of VPNB, VPCNB, and PCNVE was also tried in order to obtain the corresponding polymers with NBD moieties. However, soluble polymers were not obtained in high yield without gel production Photochem. valence isomerization of NBD moiety in poly(PNVE) and the resulting quadricyclane group in the polymer were also investigated in the film state.

IT 142246-28-4P 157716-47-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and polymerization of)

RN 142246-28-4 HCAPLUS

RN 157716-47-7 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-, (4-ethenylphenyl)methyl ester (9CI) (CA INDEX NAME)

IT 137895-90-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with chloroethyl vinyl ether and chloromethylstyrene)

RN 137895-90-0 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-, monopotassium salt (9CI) (CA INDEX NAME)

L118 ANSWER 15 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1994:410172 HCAPLUS

DN 121:10172

TI Synthesis of solar energy storage-exchange polymer containing chalcone type norbornadiene moiety and photochemical reaction of the resulting polymer

AU Kishi, Katsuhiko; Banno, Hitoshi; Kameyama, Atsushi; Nishikubo, Tadatomi

CS Fac. Eng., Kanagawa Univ., Yokohama, 221, Japan

SO Kobunshi Ronbunshu (1994), 51(5), 295-302

CODEN: KBRBA3; ISSN: 0386-2186

DT Journal

LA Japanese

GI

I (R = p-C6H4OK; R' = Ph) (II) was prepared and a polymer (III) was obtained from II and poly[p-(chloromethyl)styrene]. The photochem. activity of III was evaluated in the film state. The photochem. valence isomerization of III produced the corresponding quadricyclane (QC) groups with 60 s irradiation with a 500-W Xe lamp. The rate of photochem. valence isomerization of III polymer was higher than that of polymers based on I (R = OK; R' = Ph) or I (R = OK; R' = CONHPh) as chromophores. The reversion from the QC groups to norbornadiene (NBD) moieties in the polymers was carried out using 5,10,15,20-tetraphenyl-21H,23H-porphinecobalt(II) as a catalyst in THF solution The catalytic reversion proceeded very smoothly. The thermal reversion from QC groups to NBD moieties in the film state also proceeded smoothly.

IT 137895-90-0DP, reaction products with poly[p-

(chloromethyl) styrene]

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and photoisomerization of)

RN 137895-90-0 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-, monopotassium salt (9CI) (CA INDEX NAME)

● K

L118 ANSWER 16 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1994:323182 HCAPLUS

DN 120:323182

TI Antitumor agents II: synthesis and anticancer activity of dehydrogenated

carboncyclic analogs of norcantharidin

AU Fang, Y.; Tian, S. L.; Li, K. Q.; Zhao, S. W.; Wang, Z. Y.

CS Natl. Inst. Pharm. Res. & Dev., Beijing, 102206, Peop. Rep. China

SO Yaoxue Xuebao (1993), 28(12), 931-5 CODEN: YHHPAL; ISSN: 0513-4870

DT Journal

LA Chinese

GΙ

AB Title compds. I (R = H, alkyl, cyclohexyl, allyl, benzyl, Ph, substituted Ph) and II (R1 = Ph, substituted Ph) were prepared starting from Diels-Alder reaction of cyclopentadiene with acetylenedicarboxylic acid. II (R1 = 2-MeC6H4) showed anticancer activity comparable to that of norcantharidin.

IT 155049-76-6 155049-78-8 155049-79-9

155049-80-2 155049-81-3 155049-82-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn.and anticancer activity of)

RN 155049-76-6 HCAPLUS

CN Bicyclo[2.2.1]hept-2-ene-2-carboxylic acid, 3-

[[(phenylmethyl)amino]carbonyl] - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O \\
\parallel \\
C-NH-CH_2-Ph \\
CO_2H
\end{array}$$

RN 155049-78-8 HCAPLUS

CN Bicyclo[2.2.1]hept-2-ene-2-carboxylic acid, 3-[(phenylamino)carbonyl](9CI) (CA INDEX NAME)

RN 155049-79-9 HCAPLUS

CN Bicyclo[2.2.1]hept-2-ene-2-carboxylic acid, 3-[[(4-ethoxyphenyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

RN 155049-80-2 HCAPLUS

CN Bicyclo[2.2.1]hept-2-ene-2-carboxylic acid, 3-[[(4-methylphenyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

RN 155049-81-3 HCAPLUS

CN Bicyclo[2.2.1]hept-2-ene-2-carboxylic acid, 3-[[(2-methylphenyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

RN 155049-82-4 HCAPLUS

CN Bicyclo[2.2.1]hept-2-ene-2-carboxylic acid, 3-[[(2-chlorophenyl)amino]carbonyl]- (9CI), (CA INDEX NAME)

L118 ANSWER 17 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1994:301053 HCAPLUS

DN 120:301053

TI Fibrous materials with latent heat by solar light absorption and their manufacture

IN Kyokawa, Hiroshi

PA Japan

SO Jpn. Kokai Tokkyo Koho, 23 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE ---------_____ ______ -----JP 05311579 PΙ A2 19931122 JP 1992-139722 19920501 <--PRAI JP 1992-139722 19920501 <--OS MARPAT 120:301053

AB The title materials are prepared by coating fabrics with compns. comprising microcapsules containing norbornadiene derivs. (A) with a specified structure and catalysts and polymer binders or sandwiching mixts. of A and catalysts between a fabric and a plastic film or forming hollow sheath-core

bicomponent fibers with the core or hollow portion containing A and catalysts. The fabrics are useful for insulative garments. A fabric was coated with a composition comprising a binder and microcapsules containing 500:1 (mole ratio)

mixture of 2-carboxy-3-amido-2,5-norbornadiene and a Co compound catalyst and iso-PrOH to give a coated fabric exhibiting light absorption by sunlight and heat evolution without sunlight.

IT 155048-32-1

RL: USES (Uses)

(synthetic fibers containing or coatings on fabrics containing, for latent

heat

by solar light absorption)

RN 155048-32-1 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-(phenylamino)- (9CI) (CA INDEX NAME)

L118 ANSWER 18 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1993:518013 HCAPLUS

DN 119:118013

TI Synthesis of polymers bearing pendant norbornadiene moieties by addition reaction of poly(glycidyl methacrylate-co-methyl methacrylates) with 2,5-norbornadiene-2-carboxylic acids

AU Nishikubo, Tadatomi; Kawashima, Tatsuo; Watanabe, Sadayuki

CS Fac. Eng., Kanagawa Univ., Yokohama, 221, Japan

SO Journal of Polymer Science, Part A: Polymer Chemistry (1993), 31(7), 1659-65 CODEN: JPACEC; ISSN: 0887-624X

DT Journal

LA English

AB Polymers bearing photoresponsive norbornadiene (I) moieties were synthesized by the addition reaction of poly(glycidyl methacrylate-co-Me methacrylate)s containing pendent epoxide groups with 3-phenyl-2,5-norbornadiene-2-carboxylic acid (II), 3-[(phenyl)carbamoyl]-2,5-norbornadiene-2-carboxylic acid (IV), and 3-[(4-acetylphenyl)carbamoyl]-2,5-norbornadiene-2-carboxylic acid (IV), and 3-[(4-methoxyphenyl)carbamoyl]-2,5-norbornadiene-2-carboxylic acid (V) using Bu4NBr as a catalyst in DMF. The polymers bearing pendent II or IV moieties have higher photochem. reactivity in the film state than the polymers bearing pendent III or V moieties. Although the pendent quadricyclane (QC) group produced by the photoirradn. of the II moiety in these polymers has excellent storage stability in the film state with no catalyst at room temperature, the QC group in the polymer film with the catalyst reverts gradually to the I moiety at room temperature

TT 78941-78-3 79632-15-8 RL: USES (Uses) (esterification of glycidyl methacrylate-Me methacrylate copolymer with)

RN 78941-78-3 HCAPLUS

RN 79632-15-8 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-methoxyphenyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

L118 ANSWER 19 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1993:125298 HCAPLUS

DN 118:125298

TI Preparation of heat-resistant pendant norbornadienyl group-containing polymers as light energy-converting substance

IN Nishikubo, Tatatomi; Iizawa, Koji

PA Research Development Corp. of Japan, Japan

SO Jpn. Kokai Tokkyo Koho, 6 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PAN. CNI I									
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE				
PI	JP 04239025	A2	19920826	JP 1991-1725	19910110 <				
	JP 3083162	B2	20000904						
PRAI	JP 1991-1725		19910110	<					

AB The title polymers are prepared by introduction of norbornadiene derivs. into Me groups of poly[oxy(2,6-dimethyl-1,4-phenylene)] (I). Thus, reacting 1.5 mmol brominated I (Br 0.44 mol%) with 1.5 mmol K 3-phenylcarbamoyl norbornadiene-2-carboxylate gave a polymer showing good reproducibility under photo and thermal (160°) isomerization cycles.

IT 137895-90-0DP, reaction products with brominated
poly[oxy(dimethylphenylene)]

RL: PREP (Preparation)

(preparation of, as light energy-converting substances, heat-resistant)

RN 137895-90-0 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-, monopotassium salt (9CI) (CA INDEX NAME)

• к

L118 ANSWER 20 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1992:427466 HCAPLUS

DN 117:27466

TI Preparation of norbornadienylcarbonyloxyethyl vinyl ethers and their polymers

IN Matsumoto, Takeshi; Fukutome, Toshiyuki; Nishikubo, Tatatomi

PA Nisso Maruzen Chemical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN CNT 1

PAN.	CNT I						
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	JP 04018052	A2	19920122	JP 1990-118818	19900510 <		
	JP 2832858	В2	19981209				
PRAI	JP 1990-118818		19900510	<			
os	MARPAT 117:27466						
CT							

AB The title ethers I (X = H2C:CHOCH2CH2; R = H, CO2R1, Ph, CONR2-p-C6H4R3; R1 = Me, Et; R2 = H, Me, Et; R3 = H, Ac) are prepared from H2C:CHOCH2CH2Cl (II) and I (X = alkali metal) and (co)polymerized by reaction of the vinyl group, giving polymers for use as optical energy storage materials, optical memory devices, and photochromic materials. Refluxing 7.52 g I (X = K; R = Ph) with 31.97 g II in presence of Bu4NBr for 5 h gave 7.06 g I (R = Ph) which (4.52 g) was polymerized in PhMe in presence of BF3.Et2O and Et3N to give 91% polymer with photoisomerization capability.

IT 78941-78-3P

RL: PREP (Preparation)

(preparation and esterification with vinyloxyethyl chloride)

RN 78941-78-3 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-(9CI) (CA INDEX NAME)

IT 142246-28-4P 142246-29-5P

RL: PREP (Preparation)

(preparation of polymerizable)

RN 142246-28-4 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl], 2-(ethenyloxy)ethyl ester (9CI) (CA INDEX NAME)

RN 142246-29-5 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3[(ethylphenylamino)carbonyl]-, 2-(ethenyloxy)ethyl ester (9CI) (CA INDEX NAME)

L118 ANSWER 21 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1992:21635 HCAPLUS

DN 116:21635

TI Synthesis and solar energy storage property of polymers containing norbornadiene moieties

AU Iizawa, Takashi; Hijikata, Chikara; Nishikubo, Tadatomi

CS Fac. Eng., Hiroshima Univ., Higashi-Hiroshima, 724, Japan

SO Macromolecules (1992), 25(1), 21-6 CODEN: MAMOBX; ISSN: 0024-9297

DT Journal

LA English

AB Polymers having a pendant 3-[(p-substituted phenyl)carbamoyl]-2,5norbornadiene-2-carboxylate moiety and their model compds. were prepared
from the reaction of poly[4-(chloromethyl)styrene] and BzCl with
corresponding K salts using phase-transfer catalyst in DMF, resp. The
photochem. valence isomerization of pendant norbornadiene (NBD) to the

quadricyclane (QC) moiety proceeded smoothly in the film state or polymer solution upon irradiation by sunlight or high-pressure mercury lamp. The rate

of

isomerization was strongly affected by the substituent of the [(p-substituted phenyl)carbamoyl]-2,5-norbornadiene-2-carboxylate moiety in the polymers. The rate of photochem. reaction in the polymer solution was much higher than that of the corresponding model compds. On the other hand, the resulting QC groups in the polymer film scarcely reverted to the original NBD without any catalyst if it were kept in dark at room temperature for a long time. However, the reversion proceeded smoothly when (5,10,15,20-tetraphenyl-21H,23H-porphine)cobalt(II) was added to the polymer solution as a catalyst.

IT 137895-96-6P 137895-97-7P 137895-98-8P 137895-99-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and photoisomerization of, as model for norbornadiene-pendant polymers)

RN 137895-96-6 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 137895-97-7 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-methylphenyl)amino]carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 137895-98-8 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-methoxyphenyl)amino]carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 137895-99-9 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-chlorophenyl)amino]carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

, monopotassium salt (9CI) (CA INDEX NAME)

• K

RN 137895-91-1 HCAPLUS
CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-methylphenyl)amino]carbonyl]-, monopotassium salt (9CI) (CA INDEX NAME)

● K

RN 137895-92-2 HCAPLUS
CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-methoxyphenyl)amino]carbonyl]-, monopotassium salt (9CI) (CA INDEX NAME)

• к

RN 137895-93-3 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-chlorophenyl)amino]carbonyl]-, monopotassium salt (9CI) (CA INDEX NAME)

● K

L118 ANSWER 22 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:156259 HCAPLUS

DN 114:156259

TI Kinetic spectrophotometric determination of tetraphenylporphinecobalt(II) based on photochromism of immobilized norbornadiene

AU Kawabata, Yuji; Kumoyama, Hanako; Imasaka, Totaro; Ishibashi, Nobuhiko

CS Fac. Eng., Kyushu Univ., Hakozaki, 812, Japan

SO Analytica Chimica Acta (1991), 243(1), 97-101 CODEN: ACACAM; ISSN: 0003-2670

DT Journal

LA English

AB The Co(TPP) (H2TPP = tetraphenylporphine) is detected spectrophotometrically by its catalysis of a photochromic isomerism of 3-(phenylcarbamoyl)norbornadiene (NBD). NBD is immobilized on aminopropyl derivs. of porous glass beads, and is isomerized to a quadricyclane (QC) by UV irradiation The beads are then immersed in a solution containing Co(TPP), and

the QC is converted back to NBD by a catalytic reaction with Co(TPP). The rate constant, measured spectrophotometrically, is proportional to the concentration of Co(TPP). The detection limit of Co(TPP) is 60 μM for a reaction period of 1 h. This spectrophotometric detection can be applied repetitively without any supply of the chemical reagent, as NBD immobilized on the porous glass beads can be reisomerized to QC by UV irradiation

78941-78-3D, reaction products with aminopropyl-bonded porous glass beads in presence of condensing agents

RL: RCT (Reactant); RACT (Reactant or reagent)

(photochem. isomerization of, in (porphinato)cobalt(II) determination by catalytic spectrophotometry)

RN 78941-78-3 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-

(9CI) (CA INDEX NAME)

L118 ANSWER 23 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1988:185853 HCAPLUS

DN 108:185853

TI Preparation of enamines as prodrugs

PA Merck and Co., Inc., USA

SO Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PA	TENT I	NO.			KINI	DATE	AP	PLICATION NO.	DATE	
ΡI	JP	6203	3140			A2	19870213	JP	1986-177879	19860730	<
	EP	2140	09			A2	19870311	EP	1986-401678	19860728	<
	ΕP	2140	09			A3	19890111				
		R:	CH,	DE,	FR,	GB,	IT, LI, NL				
DD 3 T	770	1005	760	400			10050530				

PRAI US 1985-760423 A 19850730 <--

GI For diagram(s), see printed CA Issue.

AB Enamines I, II, and III (R1R2N = primary or secondary amine residues; R3, R4 = C1-6 alkyl, C6-10 aryl, C7-12 aralkyl, C3-10 cycloalkenyl, C2-20 alkenyl, mono-, di-, or triheterocyclyl containing ≥1 N, O, S.; R5 = H, C1-8 alkyl), useful as prodrugs, are prepared Treatment of 1-(N-morpholino)-1-cyclohexene with ClCO2Et gave 40% Et 2-oxocyclohexane-1-carboxylate (IV) which was treated with PhNH2 in C6H6 to afford 40.8% enamine III (R1 = H; R2 = Ph; R3 = Et; m = 4) (V). V was hydrolyzed by pig liver esterase and the products are PhNH2 and IV, vs. no hydrolysis for 4-(N-phenylamino)-3-pentene-2-one by the esterase.

IT 38778-79-9P 52909-66-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as prodrug)

RN 38778-79-9 HCAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 2-(phenylamino)-, ethyl ester (9CI) (CA INDEX NAME)

RN 52909-66-7 HCAPLUS

CN 1-Cyclopentene-1-carboxylic acid, 2-(phenylamino)-, ethyl ester (9CI) (CA INDEX NAME)

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L118 ANSWER 24 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN
AN
     1988:168043 HCAPLUS
DN
     108:168043
TI
     Photoresponsive vinyl polymer bearing norbornadiene as a pendant group
AU
     Kamogawa, Hiroyoshi; Yamada, Makoto
CS
    Dep. Appl. Chem., Yamanashi Univ., Kofu, 400, Japan
so
    Macromolecules (1988), 21(4), 918-23
     CODEN: MAMOBX; ISSN: 0024-9297
DT
     Journal
LΑ
    English
GI
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AB Homopolymers of I (R = OCH2-p-C6H4CH:CH2, NH-m-C6H4CH:CH2, NH-p-C6H4CH:CH2; R' = OMe, OCH2-p-C6H4Me, NH-m-C6H4Me, NH-p-C6H4Me) were prepared by radical polymerization, and the changes in their UV spectra upon UV irradiation under N atmospheric were studied. The norbornadiene group in the polymer

was converted to a quadricyclane group upon UV irradiation at >310 nm and was converted back to the norbornadiene group at 250 nm. Polymers bearing an amide substituent at the 2-position exhibited a higher photosensitivity in the solid state and a larger red shift in the absorption spectrum than those bearing a carboxylate substituent.

IT 113008-91-6P 113008-93-8P 113008-95-0P 113008-97-2P 113008-99-4P 113009-01-1P 113009-03-3P 113009-05-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and polymerization of)

RN 113008-91-6 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-ethenylphenyl)amino]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \hline & & \\ \hline & & \\ C-\text{OMe} \\ & & \\ \hline & & \\ \end{array}$$

RN 113008-93-8 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-ethenylphenyl)amino]carbonyl]-, (4-methylphenyl)methyl ester (9CI) (CAINDEX NAME)

RN 113008-95-0 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxamide, N-(4-ethenylphenyl)-N'-(4-methylphenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \hline & & \\ \hline & & \\ & & \\ \hline & & \\ \end{array}$$
 CH=CH₂

RN 113008-97-2 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxamide, N-(4-ethenylphenyl)-N'-(3-methylphenyl)- (9CI) (CA INDEX NAME)

RN 113008-99-4 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(3-ethenylphenyl)amino]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 113009-01-1 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(3-ethenylphenyl)amino]carbonyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ \hline C & NH \\ \hline CH = CH_2 \\ \hline O & Me \\ \end{array}$$

RN 113009-03-3 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxamide, N-(3-ethenylphenyl)-N'-(4-methylphenyl)- (9CI) (CA INDEX NAME)

RN 113009-05-5 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxamide, N-(3-ethenylphenyl)-N'-(3-methylphenyl)- (9CI) (CA INDEX NAME)

L118 ANSWER 25 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1986:608267 HCAPLUS

DN 105:208267

TI Exothermic isomerization of water-soluble quadricyclanes to norbornadienes by soluble and insoluble catalysts

AU Maruyama, Kazuhiro; Tamiaki, Hitoshi; Kawabata, Shigeki

CS Dep. Chem., Kyoto Univ., Kyoto, 606, Japan

SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1986), (4), 543-9 CODEN: JCPKBH; ISSN: 0300-9580

DT Journal

LA English

GI

AB H2O-soluble quadricyclanes I (R = Me, Ph) were stable in aqueous Na2CO3 solution,

but addition of a catalytic amount of a H2O-soluble Co porphyrin complexes induced

rapid and quant. isomerization of I to norbornadiene derivs. II with release of heat. Insol. catalysts prepared by adsorption of Co-TPP or Co-Pc (TPP = 5,10,15,20-tetraphenylporphyrin diamion; Pc = phthalocyanine diamion) on activated C were as active as the soluble analogs. They retained their activity after use, and could be recycled.

IT 78941-78-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, by cobalt porphyrin-catalyzed isomerization of quadricyclane)

RN 78941-78-3 HCAPLUS

L118 ANSWER 26 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1986:450862 HCAPLUS

DN 105:50862

TI Electrochemical conversion of a quadricyclane to a norbornadiene

IN Gassman, Paul G.; Hershberger, James W.

PA University of Minnesota, USA

SO U.S., 6 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.C	NT 1						
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI	US 4582578	Α	19860415	US 1985-762111	19850802 <		
	CA 1277949	A1	19901218	CA 1986-514209	19860718 <		
	IL 79475	A1	19910816	IL 1986-79475	19860721 <		
	AU 8660461	A1	19870205	AU 1986-60461	19860723 <		
	AU 596045	B2	19900412				
1	JP 62063693	A2	19870320	JP 1986-179813	19860730 <		
PRAI	US 1985-762111	Α	19850802	<			

AB A method for the electrochem. isomerization of a quadricyclane to a norbornadiene with the net release of thermal energy comprises: (a) forming an electroconductive solution comprising quadricyclane and a neutral carrier oxidant compound such as a triarylamine; (b) oxidizing the carrier oxidant compound to the corresponding cation radical by applying an anodic potential to the solution; (c) oxidizing quadricyclane to the corresponding quadricyclane radical by means of a single electron transfer from quadricyclane to the cation radical of the oxidant compound, in which the quadricyclane radical spontaneously isomerizes to the norbornadiene radical with the liberation of thermal energy; and (d) reducing the norbornadiene cation radical to the corresponding norbornadiene with the liberation of thermal energy. The isomerization reaction can be stopped instantly by the application of a cathodic potential and restarted by reapplication of the anodic potential, and systems employing this reaction can be used for solar energy storage and release.

IT 78941-78-3P

RL: PREP (Preparation)

(preparation of, electrochem., from the corresponding quadricyclane)

RN 78941-78-3 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-(9CI) (CA INDEX NAME)

L118 ANSWER 27 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1986:148368 HCAPLUS

DN 104:148368

TI Development of a solar energy storage process. Photoisomerization of a norbornadiene derivative to a quadricyclane derivative in an aqueous alkaline solution

AU Maruyama, Kazuhiro; Tamiaki, Hitoshi; Kawabata, Shiqeki

CS Fac. Sci., Kyoto Univ., Kyoto, 606, Japan

SO Journal of Organic Chemistry (1985), 50(24), 4742-9 CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 104:148368

GΙ

AB Aqueous alkaline norbornadiene derivs. I (R = R1 = H, Me; R = H, R1 = Me, PhCH2,

CMe3, Ph; RNR1 = pyrrolidino) are quant. valence isomerized to the corresponding quadricyclanes II, in air, on irradiation by sunlight. The cyclopropane and cyclobutane rings of II are usually reactive with H2O; this is not observed here but I (R = Me, R1 = Ph, R = R1 = Ph; RNR1 = indolino) give undesirable compds. under these conditions. The linked analogs III, IV, and V of I are also prepared; they are as photoreactive as I and have increased solubility and higher heat storage ability than I. These compds. are potentially useful for solar energy storage.

IT 78941-78-3

RL: PROC (Process)

(UV and photoisomerization of)

RN 78941-78-3 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl](9CI) (CA INDEX NAME)

IT 79632-15-8 96627-81-5 96627-82-6

RL: PROC (Process)

(photoisomerization of)

RN 79632-15-8 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-methoxyphenyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

RN 96627-81-5 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-chlorophenyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

RN 96627-82-6 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-methylphenyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

IT 98736-24-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and photochem. isomerization of)

RN 98736-24-4 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3[[(phenylmethyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

IT 84293-21-0P 84293-22-1P 98736-27-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and photoisomerization of)

RN 84293-21-0 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3,3'-[1,2-phenylenebis(iminocarbonyl)]bis- (9CI) (CA INDEX NAME)

RN 84293-22-1 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3,3'-[1,4-phenylenebis(iminocarbonyl)]bis- (9CI) (CA INDEX NAME)

RN98736-27-7 HCAPLUS

Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-CN[(methylphenylamino)carbonyl] - (9CI) (CA INDEX NAME)

L118 ANSWER 28 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1985:220277 HCAPLUS

DN 102:220277

ΤI Valence isomerization between water-soluble norbornadiene and quadricyclane derivative

ΑU Maruyama, Kazuhiro; Tamiaki, Hitoshi; Yanai, Tetsuya

CS Fac. Sci., Kyoto Univ., Kyoto, 606, Japan

SO Bulletin of the Chemical Society of Japan (1985), 58(2), 781-2 CODEN: BCSJA8; ISSN: 0009-2673

DTJournal

English LΑ

GΙ

RN

$$CONH$$
 R
 CO_2H
 I
 CO_2H
 II

AB Photoisomerization of norbornadienecarboxylic acids I (R = H, Cl, Me, MeO) to the corresponding quadricyclanes II (same R) in aqueous-alkaline solution

was clean and dependent on the para substitution of the aryl group. Rate consts. for the Co 5,10,15,20-tetrakis(p-carboxyphenyl)porphyrin-catalyzed valence isomerization II → I were determined

78941-78-3 79632-15-8 96627-81-5 IT

96627-82-6

RL: RCT (Reactant); RACT (Reactant or reagent) (photochem. valence isomerization of)

78941-78-3 HCAPLUS

Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-CN

(9CI) (CA INDEX NAME)

RN 79632-15-8 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-methoxyphenyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

RN 96627-81-5 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-chlorophenyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

RN 96627-82-6 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4methylphenyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

L118 ANSWER 29 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1984:423039 HCAPLUS

DN 101:23039

TI Acceleration of valence isomerism

PA Nard Institute Ltd., Japan; Maruyama, Kazuhiro

SO Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

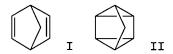
PATENT NO.

KIND DATE

APPLICATION NO.

DATE

PI JP 59020261 A2 19840201 JP 1982-129150 19820724 <-JP 03015626 B4 19910301
PRAI JP 1982-129150 19820724 <-GI



AB Norbornadiene (I) or its derivs. having substituents at position 2,3,5, or 6 were prepared by valency isomerism of quadricyclane (II) or its derivs. in the presence of metal complexes of H2O-soluble porphyrins or phthalocyanines. Thus, an aqueous mixture of 10.5 mg 3-phenylcarbamoylquadricyclane-2-carboxylic acid and 0.21 mol Na2CO3 was kept at ordinary temps. in the presence of Co complex of hematoporphyrin to give 10.5 mg 3-phenylcarbamoylnorbornadiene-2-carboxylic acid. Ten addnl. norbornadienes were similarly prepared

TT 78941-78-3P 79632-14-7P 79632-15-8P 79632-18-1P 79632-19-2P 84293-22-1P 90687-79-9P

RN 78941-78-3 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-(9CI) (CA INDEX NAME)

RN 79632-14-7 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(1-naphthalenylamino)carbonyl]- (9CI) (CA INDEX NAME)

RN 79632-15-8 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-methoxyphenyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

RN 79632-18-1 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 79632-19-2 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxamide, N,N'-diphenyl- (9CI) (CA INDEX NAME)

RN 84293-22-1 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3,3'-[1,4-phenylenebis(iminocarbonyl)]bis- (9CI) (CA INDEX NAME)

RN 90687-79-9 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxamide, N-1-naphthalenyl- (9CI) (CA INDEX NAME)

L118 ANSWER 30 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1984:5941 HCAPLUS

DN 100:5941

TI Valence isomerization between norbornadienes and quadricyclanes

PA Maruyama, Kazuhiro, Japan; Nado Kenkyusho, Ltd.

SO Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

1141	C11 1 1						
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	JP 58110550	A2	19830701	JP 1981-214186	19811224 <		
	JP 02017535	B4	19900420				
PRAI	JP 1981-214186		19811224	<			

AB Norbornadienes I (R = Ph, p-methoxyphenyl, 1-naphthyl, CMe3; R1 = OH, OMe, NHPh), II (R = Ph, 1-naphthyl), or III (Z = p-phenylene, CH2CH2) underwent photochem. isomerization to corresponding quadricyclanes, e.g. IV. This required no photosensitizer and the isomerization was reversed with Rh2(CO)4Cl2 or by pyrolysis. Thus, norbornadiene-2,3-dicarboxylic anhydride treated with equimol. PhNH2 in CH2Cl2 at 0° gave 93% I (R = Ph, R1 = OH), which was dissolved in MeCN and exposed to a 300-W high-pressure Hg lamp for 5-20 h to give .apprx.100% IV.

IT 78941-78-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and valence isomerization of)

RN 78941-78-3 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-(9CI) (CA INDEX NAME)

IT 79632-14-7P 79632-15-8P 79632-18-1P

79632-19-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 79632-14-7 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(1-naphthalenylamino)carbonyl]- (9CI) (CA INDEX NAME)

RN 79632-15-8 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4methoxyphenyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

RN 79632-18-1 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 79632-19-2 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxamide, N,N'-diphenyl- (9CI) (CA INDEX NAME)

L118 ANSWER 31 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1983:57162 HCAPLUS

DN 98:57162

TI A water-soluble solar energy storage system

AU Maruyama, Kazuhiro; Tamiaki, Hitoshi

CS Fac. Sci., Kyoto Univ., Kyoto, 606, Japan

SO Chemistry Letters (1982), (11), 1699-702

CODEN: CMLTAG; ISSN: 0366-7022

DT Journal

LA English

AB In an alkaline aqueous solution, photochem. valence isomerization of norbornadiene

derivs. to quadricyclane derivs. occurred quant., and reverse isomerization under release of heat was achieved by catalytic action of Co hematoporphyrin [29497-66-3] and analogs. This system may be of great practical use for solar-energy storage.

IT 78941-78-3 84293-21-0 84293-22-1

RL: PROC (Process)

(for solar energy storage, photoisomerization of, cobalt hematoporphyrin and analogs in)

RN 78941-78-3 HCAPLUS

RN 84293-21-0 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3,3'-[1,2-phenylenebis(iminocarbonyl)]bis- (9CI) (CA INDEX NAME)

RN 84293-22-1 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3,3'-[1,4-phenylenebis(iminocarbonyl)]bis- (9CI) (CA INDEX NAME)

L118 ANSWER 32 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1982:162225 HCAPLUS

DN 96:162225

TI Paramagnetically induced NMR shifts. IX. Syntheses and properties of highly substituted vinamidines

AU Knorr, Rudolf; Weiss, Alfons

CS Inst. Org. Chem., Univ. Muenchen, Munich, D-8000/2, Fed. Rep. Ger.

SO Chemische Berichte (1982), 115(1), 139-60 CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

OS CASREACT 96:162225

AB R1NLiCR2:CHR3 [R1 = Ph, 3,5-Me2C6H3; R2 = Me, Et, Pr, CMe3, pentyl, Ph; R3 = Me, 1-cyclohexen-1-yl, (un)substituted Ph, Et, 1-naphthyl, PhO, PhS, H, Bu, CH:NPh; R2R3 = (CH2)n (n = 3,4,5,6,10), CH2CH2CHMeCH2, o-C6H4CH2CH2, o-C6H4CH2, bicyclo[2.2.2]oct-2-en-2-yl and 2,5-diene isomers], prepared in situ from R1N:CR2CH2R3, (Me2CH)2NH, and MeLi, reacted with R4R5C:NR1 (R4 = H, Me, CMe3, Et, Pr, Ph; R5 = alkoxy, Cl) to give vinamidines R1NHCR2:CR3CR4:NR1, R1N:CR2CR3:CR4NHR1.HClO4, and R1N:CR2CR3:CR4NHR1 or their tautomers R1N:CR2CH3CR4:NR1. This α-iminoalkylation corresponds in its regioselectivity to the anionization of R1N:CR2CH2R3. N-Acylations to give amidine derivs. are competing reactions and secondary reactions may lead to triacyl methanes, such as PhNHCEt:C(CH:NPh)CH:NPh, PhNHCH:C(CEt:NPh)CH:NPh, PhNHCH:C(COEt)CH:NPh, and PhNHCH:C(CH:NPh)CH:NPh. The tautomeric and conformational equilibrium of the products are substituent dependent.

IT 81067-15-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrogenation of)

RN 81067-15-4 HCAPLUS

CN Bicyclo[2.2.2]octa-2,5-dien-2-amine, N-phenyl-3-[(phenylimino)methyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

IT 81067-16-5P 81067-21-2P

RN 81067-16-5 HCAPLUS

CN Bicyclo[2.2.2]octa-2,5-dien-2-amine, N-phenyl-3-[(phenylimino)methyl]-, (E)-, monoperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 81067-15-4 CMF C21 H20 N2

Double bond geometry as shown.

CM 2

CRN 7601-90-3 CMF Cl H O4

RN 81067-21-2 HCAPLUS

CN Bicyclo[2.2.2]oct-2-en-2-amine, N-phenyl-3-[(phenylimino)methyl]-, (E)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

L118 ANSWER 33 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN AN 1981:606796 HCAPLUS DN 95:206796 TI Exploitation of solar energy storage systems. Valence isomerization between norbornadiene and quadricyclane derivatives ΑU Maruyama, Kazuhiro; Terada, Kazutoshi; Yamamoto, Yoshinori CS Fac. Sci., Kyoto Univ., Kyoto, 606, Japan SO Journal of Organic Chemistry (1981), 46(26), 5294-300 CODEN: JOCEAH; ISSN: 0022-3263 DT Journal LA · English AΒ The use of Cu(I)-N ligand catalysts such as Ph3PCuCl·L (L = 2,2'-bipyridine, o-phenanthroline, phthalazine) and Ph3PCuBr·pyridine [25753-77-9] enables the photochem. isomerization of norbornadiene to quadricyclane to occur at longer wavelengths than 350 nm, at which the CuCl catalyst itself cannot induce such an isomerization. Among the norbornadiene derivs. bearing various chromophores, 3-(phenylcarbamoyl)norbornadiene-2-carboxylic acid (I) 78941-78-3] undergoes a facile and quant. isomerization into the corresponding quadricyclane derivative (II) in sunlight. The back-isomerization of II to I proceeds quant. by the use of catalytic amts. of Rh2(CO)4Cl2. 78941-78-3P 79632-14-7P 79632-15-8P IT 79632-18-1P 79632-19-2P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and photoisomerization of, for solar energy storage) RN 78941-78-3 HCAPLUS

Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl]-

(CA INDEX NAME)

CN

RN 79632-14-7 HCAPLUS
CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(1-naphthalenylamino)carbonyl]- (9CI) (CA INDEX NAME)

RN 79632-15-8 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[[(4-methoxyphenyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

RN 79632-18-1 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, 3-[(phenylamino)carbonyl], methyl ester (9CI) (CA INDEX NAME)

RN 79632-19-2 HCAPLUS

CN Bicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxamide, N,N'-diphenyl- (9CI) (CA INDEX NAME)

L118 ANSWER 34 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1981:514505 HCAPLUS

DN 95:114505

TI Highly efficient valence isomerization between norbornadiene and quadricyclane derivatives under sunlight

AU Maruyama, Kazuhiro; Terada, Kazutoshi; Yamamoto, Yoshinori

CS Fac. Sci., Kyoto Univ., Kyoto, 606, Japan

SO Chemistry Letters (1981), (7), 839-42

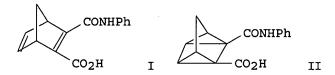
CODEN: CMLTAG; ISSN: 0366-7022

DT Journal

LA English

OS CASREACT 95:114505

GΙ



AB 3-(N-Phenylcarbamoyl)-2,5-norbornadiene-2-carboxylic acid (I) undergoes a facile and quant. isomerization to the corresponding quadricyclane derivs. II in sunlight. The back isomerization of II to I proceeds quant. in the presence of catalytic amts. of Rh2(CO)4Cl2.

IT 78941-78-3

RL: RCT (Reactant); RACT (Reactant or reagent)
 (photochem. isomerization of)

RN 78941-78-3 HCAPLUS

L118 ANSWER 35 OF 35 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1977:502009 HCAPLUS

DN 87:102009

TI 2-Aminocycloalkanecarboxylic acids and their derivatives

IN Bernath, Gabor; Gera, Lajos; Dondos, Gyorgy; Kovacs, Kalman; Janvari, Erzsebet; Sebestyen, Gyula; Ecsery, Zoltan; Hermann, Judit

PA Chinoin Gyogyszer es Vegyeszeti Termekek Gyara Rt., Hung.

SO Ger. Offen., 34 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	DE 2624290	A1	19770414	DE 1976-2624290	19760531 <
	HU 19947	0	19810528	HU 1975-CI1580	19750602 <
	HU 177576	P	19811128		
	CS 217955	P	19830225	CS 1976-3591	19760528 <
	CS 217955	В	19830225		
	AT 350518	В	19790611	AT 1976-3954	19760531 <
	AT 7603954	Α	19781115		

•	FR	2313023	1	A1	19761231	FR	1976-16648	19760602	<
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	ΑT	352099]	3	19790827	AT	1977-6126	19770824	<
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GI									

$$COR$$
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AB The title compds., cis and trans-I (R = OH, OEt, NHPh, NHBu, etc; R1 = H, CO2CH2Ph, CHO, Ac, Me, etc; R2 = H, Me; n = 1, 2) were prepared Thus, Et 2-oxocyclohexanecarboxylate reacted with PhNH2, followed by hydrogenation, to give II (R = Et), which was hydrolyzed to II (R = H). I are useful as analgesics, antipyretics, and anesthetics (no data).

IT 38778-79-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrogenation of)

RN 38778-79-9 HCAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 2-(phenylamino)-, ethyl ester (9CI) (CA INDEX NAME)

=> d his

(FILE 'HCAPLUS' ENTERED AT 12:26:37 ON 19 APR 2005) DEL HIS L1 3 S US20040176458/PN OR (US2003-736711# OR US2002-435258#)/AP,PRN E LEBAN J/AU L260 S E3-E5, E7-E10 E KRALIK M/AU L3 120 S E3, E4 E 4SC/PA,CS 24 S E3-E20 L4E 4 SC/PA, CS L5 2 S E5-E12 E 4S C/PA,CS E 4 S C/PA, CS L6 3 S L1 AND L2-L5 L7 194 S L2-L5 NOT L6

SEL RN L6

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L82
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L83
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L86
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L88
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L90
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L91
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L92
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L93
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L94
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L100
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L104
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L105
             89 S L104 AND P/DT
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                SEL HIT RN
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L110
             22 S L110 AND (PY<=2002 OR PRY<=2002 OR AY<=2002)
L111
L112
             10 S L111 AND P/DT
L113
             8 S L112 NOT HERBICID?
             23 S L106 NOT L107
L114
                SEL HIT RN
     FILE 'REGISTRY' ENTERED AT 14:20:44 ON 19 APR 2005
L115
           330 S E219-E548
     FILE 'HCAPLUS' ENTERED AT 14:21:57 ON 19 APR 2005
L116
             38 S L84, L113
L117
             3 S L116 AND L1-L7
L118
             35 S L116 NOT L117
     FILE 'REGISTRY' ENTERED AT 14:22:31 ON 19 APR 2005
     FILE 'HCAPLUS' ENTERED AT 14:22:45 ON 19 APR 2005
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